

NATIONAL HIGH MAGNETIC FIELD LABORATORY

REPORTS



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HYBRID MAGNET RETURNS TO 45 T

— & —
NMR Spectroscopy
and Imaging

Multi-Institutional
Synthetic Materials
Project

In-House Research
Program Goes Online

Diphtheria Toxin
Repressor Proteins

Open House 2001



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From the Director's Desk

Jack Crow

In the Fall Issue of NHMFL Reports, I announced that the National Science Board had approved \$117.5 million in funding for the NHMFL through 2005. This award represents a 35 percent increase over the last five-year grant of \$87.5 million (1995-2000), so we were generally pleased. It is important to note that the level of support is not the same each year (funding profile: FY 2000, \$20 M; FY 2001, \$23.5 M; FY 2002, \$24 M; FY 2003, \$24.5 M; and FY 2004, \$25.5 M) and will depend on successful annual reviews, scientific progress, and availability of funds.

Recently, I e-mailed the NHMFL users community and asked you to contact your United States Congressman and Senators regarding the inadequate level of funding for the National Science Foundation in the President's budget request for FY 2002. If you have not contacted them yet, I urge you to do so immediately. The President's FY 2002 budget sent to Congress recently requested a meager increase of 1.3% for NSF, compared to a 14% increase last year. If the President's budget were enacted, the Directorate for Materials Research would receive an overall cut of \$4.33 million or a 2.1% decrease. Furthermore, the budget for materials research would decline by 4.9% or by \$8.83 million, which constitutes a lot of individual research grants that we all seek to obtain. The NSF is even anticipating the new administration to cut the NSF budget next year for FY 2003. As mentioned above, the NHMFL is projected to receive an accelerated budget over the next four years, however, the laboratory's budget is heavily dependent on Congress appropriating adequate funds for NSF.

It is vitally important that Congress hear from our scientific community. For too long, we have been reticent in making our view known in the corridors of government on the importance of basic research to society and the economy. If we do not become more proactive, rest assured that future budgets for research will continue to decline and the more aggressive groups will reap our losses. This need to aggressively pursue our respective Congressmen to support basic science research and the NSF, in particular, may

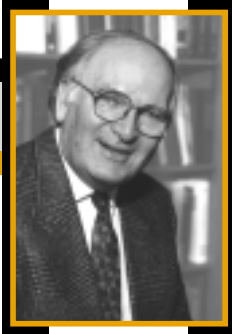
become a biannual responsibility. First, at this time when Congress is considering authorization bills, and later in the year, when they pursue actual appropriation bills.

Many economists and Alan Greenspan frequently acknowledge that the economic prosperity of the last several years can be attributed to the nation's investments in research and development made decades ago. The fruits of basic research are also vital in educating and training our next generation of scientific leaders.

President Bush proclaimed that he wants to double the budget for the National Institutes of Health (NIH). There are many in Congress, however, who would like to double the NSF budget over five years. We must show our support for this initiative and elevate the awareness and importance of basic research. Even the new chairman of the House Science Committee, Representative Sherwood Boehlert, recognizes the growing concern over the fact that the NIH budget is growing "far faster" than any other science agency.

I hope that you will take a few minutes out of your busy schedules and write your Congressional delegation. Many of you may think that one more letter or e-mail will make no difference. Nothing could be further from the truth—Congress is merely a reflection of the general public—voices *do* count. Those of us in Florida learned the importance of every vote last November.

Jack Crow



From the Chief Scientist's Desk

J. Robert Schrieffer

Recently, the structure of the In-House Research Program (IHRP) underwent changes that are intended to make it more responsive to proposers and improve the expertise in judging the proposals. We hope the new arrangements will provide an improved operation of the IHRP.

NSF Objectives. In 1996, The National Science Foundation (NSF) charged the NHMFL with developing an in-house research program that:

- utilizes the NHMFL facilities to carry out high quality high field research at the forefront of science and engineering; and
- advances the NHMFL facilities and their scientific and technical capabilities.

To this end, the NHMFL has envisioned an in-house research program that not only guides and stimulates magnet and facility development, but additionally provides intellectual leadership for experimental and theoretical research in magnetic materials and phenomena. The IHRP seeks to achieve these objectives through funded research projects of normally one to two years duration in the following categories:

- small, seeded collaborations between internal and/or external investigators that utilize their complementary expertise to enhance the capabilities of the NHMFL;
- bold, but risky efforts that hold significant potential to extend the range and type of experiments; and
- initial seed support for new faculty and research staff targeted to magnet laboratory enhancements.

The 2001 solicitation was announced March 9, 2001, with a pre-proposal deadline of April 6, 2001.

Research Program Committee.

In order to enhance the programs' review process, the NHMFL has restructured its Research Program Committee (RPC). The RPC is charged to provide guidance to the NHMFL on new research programs, facility development needs, and to serve as the primary review body for proposals submitted to the IHRP. In meeting the charge given by the NSF, the NHMFL has three primary research areas representing the activities pursued at the laboratory. They include: Condensed Matter Sciences, Biological and Chemical Sciences, and Magnet and Magnet Materials Development.

The RPC has been restructured to be more responsive to these areas. The RPC will be chaired by the IHRP Director and will be composed of three subcommittees representing each area noted above. Membership on the committee will be balanced to provide equitable representation from the three participating institutions, and will also include appropriate representation from the external user community.

Online IHRP Submission & Review Process.

To make it easier for principal investigators (PIs) and reviewers, the IHRP's submission and review process went online this year at <http://ihrp.magnet.fsu.edu>. The deadline for pre-proposal submissions was April 6; the deadline for pre-proposal reviews was April 30.

The pre-/full proposals will be reviewed by the appropriate subcommittee of the RPC designated by the submitter of the proposal. The review criteria for pre-/full proposals are:

1. Research performance competence
This criterion relates to the capability of the investigator(s), the technical soundness of the proposed research, and the adequacy of the institutional resources available.
2. Intrinsic merit of the research
This criterion is used to assess the likelihood that the research will lead to new discoveries, fundamental

advances in the fields of high magnetic field science or engineering, or have substantial impact on progress in those fields.

3. Utility or relevance of the research to the NHMFL mission

This criterion is used to assess the likelihood that the research can contribute to the achievement of the NHMFL IHRP objectives, and thereby, serve as the basis for driving, enhancing, or improving the NHMFL user facilities, capabilities, or expertise.

4. Effect of the research on the infrastructure of high magnetic field science and engineering

This criterion relates to the potential of the proposed research to contribute to better understanding or improvement of the quality, distribution, or effectiveness of the nation's high magnetic field scientific and engineering research, education, and manpower base.

The review process for the Condensed Matter and Biological and Chemical Subcommittees is as follows:

- The six internal members of the applicable subcommittee (the two members each from FSU, UF and LANL) will review pre-proposals and rank them based on scientific merit and facility impact.
- The Directors of the User Programs will review pre-proposals with an emphasis on facility impact.
- The subcommittees will report their review results to the IHRP Director and Chief Scientist who will select the pre-proposals that will go forward to full proposals.
- The full subcommittee (including all nine members) will review and rank full proposals.
- The review results of the full subcommittee will be reported to the IHRP Director and Chief Scientist who will review the rankings of the full proposals; the Chief Scientist will then select the proposals to be funded.

The review process for the Magnet and Magnet Materials Technology subcommittee is as follows:

- The full subcommittee, including the ex-officio members, will review and rank the pre-proposals based on scientific merit and facility impact.
- The Directors of User Programs will review pre-proposals with an emphasis on facility impact.
- The subcommittee will report their review results to the IHRP Director and Chief Scientist who will select the pre-proposals that will go forward to full proposals.
- The full subcommittee, including the ex-officio members will review and rank full proposals.
- The review result of the full subcommittee will be reported to the IHRP Director and the Chief Scientist who will review the rankings of the full proposals; the Chief Scientist will then select the proposals to be funded.

The RPC subcommittees select the pre- and full proposals that meet the review criteria, keeping in mind that the funded projects must be of highest quality. The RPC subcommittees will share their review comments with the PI(s) so that he/she can consider their comments. The NHMFL reserves the right to turn down pre-/full proposals that do not fully meet the solicitation guidelines.

The NHMFL IHRP strongly encourages collaboration across host-institution boundaries and between internal and external investigators in academia, national laboratories, and industry, as well as interaction between theory and experiment. Projects are also encouraged to drive new or unique research, i.e., serve as seed money to develop initial data leading to external funding of a larger program. In accord with NSF policies, the NHMFL cannot fund clinical studies.

NHMFL Research Program Committee

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Albert Migliori

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2. FSU	Dragana Popovic
3. UF	Kevin Ingersent
4. UF	Mark Meisel
5. LANL	Marty Maley
6. LANL	Neil Harrison
7. External User	Craig Taylor (University of Utah)
8. External User	Dimitri Basov (University of CA, San Diego)
9. External User	Steve Hill (Montana State University)

Biological and Chemical Sciences Subcommittee

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2. FSU	Tim Logan
3. UF	Alex Angerhofer
4. UF	Steve Blackband
5. LANL	Tom Terwilliger
6. LANL	Cliff Unkefer
7. External User	Warren Warren (Princeton University)
8. External User	Les Butler (Louisiana State University)
9. External User	Sandra Eaton (University of Denver)

Magnet and Magnet Materials Technology Subcommittee

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2. UF	Anthony Brennan
3. LANL	Jim Sims
4. Director MS&T	Steve Van Sciver (Ex-officio)
5. Deputy Director	Hans Schneider-Muntau (Ex-officio)

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1. DC Field	Bruce Brandt
2. NMR	Tim Cross
3. ICR	Alan Marshall
4. EMR	Louis-Claude Brunel

UF

1. MRI	Steve Blackband
2. High B/T	Jian-sheng Xia
3. Brain Institute	William Luttge

LANL

1. Pulsed Field	Alex Lacerda
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NHMFL Hybrid Magnet is Again at 45 T!

On February 1, 2001, the NHMFL Hybrid Magnet was returned to user service at 45.1 T after nearly seven months of operation at reduced field strength.

The first user to operate at 45 T DC was John Singleton of Oxford University. The experiment examined the magnetoresistance of the prototype layered organic superconductor κ -(BEDT-TTF)₂Cu(NCS)₂ (Fig. 1). There has been vigorous debate in the scientific community about the nature of the superconductivity in this material and whether the interlayer electrical transport is coherent or incoherent.

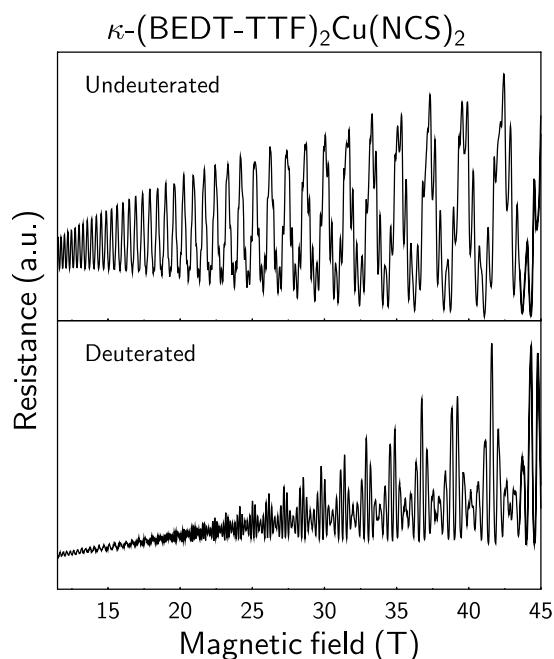
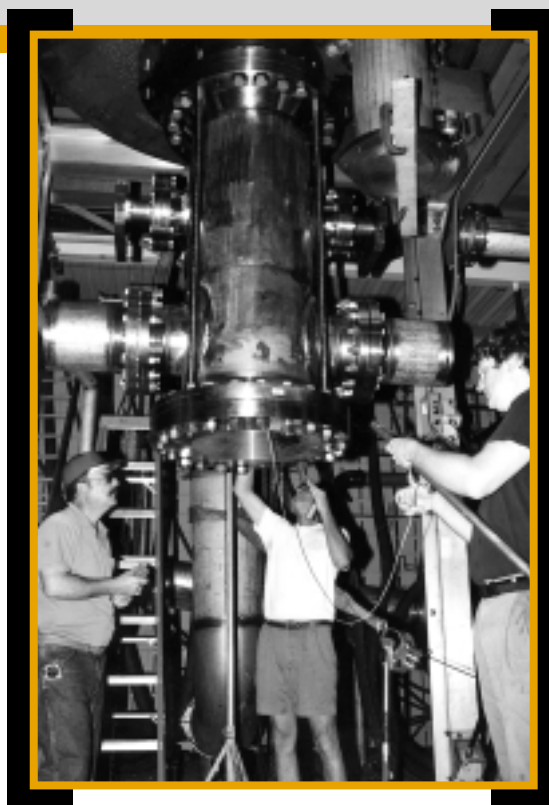


Figure 1. Magnetoresistance of κ -(BEDT-TTF)₂Cu(NCS)₂ versus applied magnetic field.

Singleton *et al.* used the Hybrid Magnet to exceed the upper critical magnetic field of 35 T in their sample. Using a two-axis rotation probe, they measured the normal state magnetoresistance as a function of magnetic field orientation. The appearance of a peak in the magnetoresistance when the magnetic field lies parallel to the sample layers is a very strong indication that the Fermi surface of this material is three dimensional and that the electrical transport between the layers is coherent.

Fig. 2 shows the magnetoresistance at 42 T, as a function of polar angle, θ , at two azimuthal orientations, Φ . The



coherence peak is visible close to $\theta=0$ degrees; conventional angle-dependent magnetoresistance oscillations can be seen on either side.

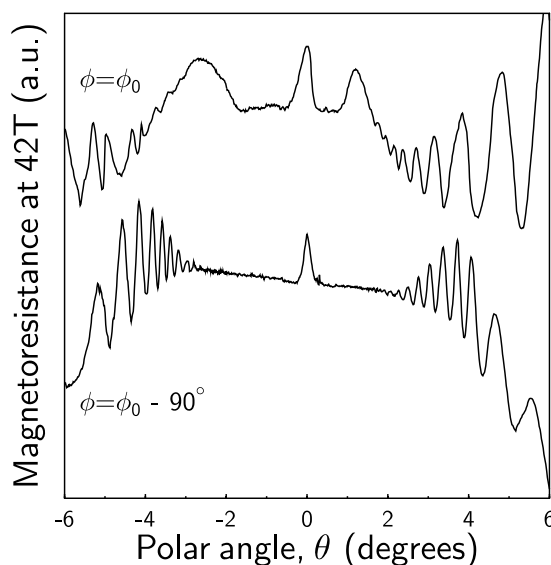


Figure 2. Magnetoresistance of κ -(BEDT-TTF)₂Cu(NCS)₂ versus polar angle.

The NHMFL Hybrid is the highest field DC magnet in the world and the only facility in which this experiment could be performed. The Hybrid consists of two sets of coils: the superconducting outsert and the resistive insert. The outsert contains three concentric cable-in-conduit coils operating at 1.8 K. The resistive insert contains five water-cooled Florida-Bitter coils. The system was originally designed for the outsert to provide 14.2 T with 30.8 T coming from the insert for a total of 45.0 T.

On July 7, 2000, the superconducting outsert was damaged during an unprotected quench. Since that time, it has been operating at 80% of its design field, i.e., 11.4 T. In December 2000, an upgrade of the resistive insert was completed that allowed operation of the insert at sufficiently high field to overcome the shortfall from the outsert, i.e., 33.7 T. On February 1 and 2, 2001 the combined system was operated to 45.1 T for a total of 13 full field sweeps over a nine-hour period. This accomplishment makes the magnet not only the highest field DC magnet in the world, but the insert by itself is the highest field resistive magnet in the world.

The upgrade of the resistive insert constitutes a substantial advance in high field resistive magnet design. Traditionally, high field resistive magnet designers have focused on the stress state at the mid-plane of the magnet, and ignored end effects. It was argued that since the field is a maximum at the mid-plane, the stress must be a maximum at the mid-plane. If one examines the stress in a hybrid insert carefully, one sees that the discontinuity of the helical structure coupled with the lack of magnetic clamping at the end of the coil can lead to a large in-plane bending of the end disks. Consequently, hybrid inserts have frequently been limited by disk bending at the ends of the coils rather than hoop tension at the mid-plane. To address this problem, it has been common practice at various laboratories to use thicker turns at the ends of the coils than the mid-plane.

The recent upgrade to the NHMFL Hybrid is the first time magnet designers have considered the stress state at the mid-plane and ends separately and used disks with different cooling hole patterns at different points in the coil to best

accommodate the local stress state. Fig. 3 shows the cooling hole pattern used at the mid-plane and ends of the innermost coil of the hybrid insert. The mid-plane cooling hole pattern uses very long slender holes to maximize the hoop strength of the disk. The end turns use shorter, broader holes, which results in an in-plane bending stiffness nearly 30 times greater than at the mid-plane. By varying the cooling hole pattern along the length of the coil, we are able to provide a coil with a more uniform stress state and higher operating field: perhaps 48 to 50 T at some future date.

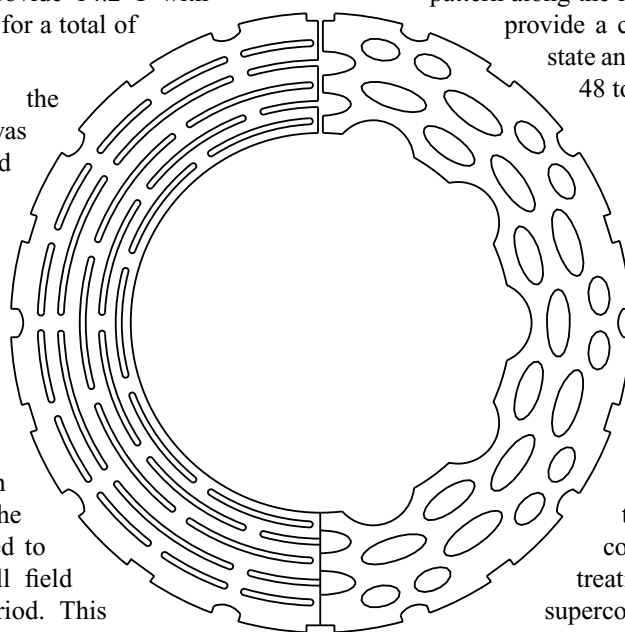
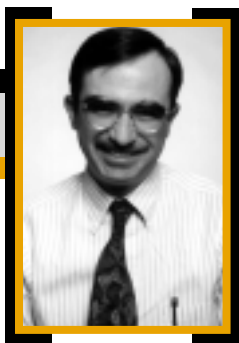


Figure 3. Cooling hole patterns of Florida-Bitter disks of innermost coil of hybrid insert. Left side is mid-plane hole pattern: long slender holes maximize hoop strength. Right side is end-turn pattern: shorter, broader holes maximize in-plane bending stiffness.

Per the NSF's mandate, the NHMFL intends to repair the superconducting outsert by replacing the damaged *A* coil. This repair project will be led by John Miller and will require the following steps: (1) procuring un-reacted Nb₃Sn cable, (2) installing the cable in a stainless steel jacket, (3) insulating the jacketed conductor with glass tape, (4) winding the jacketed conductor into a coil, (5) heat treating the coil to form the Nb₃Sn superconductor, (6) making terminals, (7) disassembling the existing outsert, (8) installing the new coil, and (9) testing. The plan is to perform tasks two through nine in-house. The project is intended to take about three years, assuming funding is available.

Until the new super-conducting *A* coil is ready for installation, the Hybrid will be available to the user community at 45 T. Additional improvements to the insert are presently underway to further enhance the end turn stiffness of the coils, thereby increasing the lifetime at these increased currents and fields. After the outsert has been replaced, we intend to push the combined system toward 50 T by making additional minor improvements to the resistive insert. The Hybrid is expected to have annual maintenance shutdowns lasting a few months. The 2001 shutdown is scheduled from February 5 until May 28.

This article was contributed by Mark Bird, Arzhang Ardavan, Hans Schneider-Muntau, and John Miller. For more information, contact Mark Bird via e-mail (bird@magnet.fsu.edu).



ATTENTION USERS

Timothy Cross
Director, NMR Spectroscopy and Imaging Program

NHMFL NMR Spectroscopy and Imaging Update

This program has a mission to develop technology and applications at the highest magnetic fields through both in-house and external user activities. This is a very broad mission in solution and solid-state NMR spectroscopy as well as imaging and diffusion measurements. Unique capabilities are being developed in all of these arenas using superconducting magnets up to 19.6 T and resistive magnets up to 25 T or 1.066 GHz. Condensed matter NMR has extended this range up to 45 T in the hybrid magnet at the NHMFL. These magnets vary from very narrow bore (31 mm) to whole body dimensions, and they are located at two sites—the NHMFL in Tallahassee and at the UF McKnight Brain Institute in Gainesville. Here, we highlight two new capabilities made possible by the efforts of Ago Samosan from the National Institute of Chemical and Biophysics in Estonia and Andrei Samoilenko from the Chemical and Physics Institute, Russian Academy of Sciences in collaboration with Zhehong Gan, Bill Brey, Riqiang Fu, and Peter Gor'kov at the NHMFL. Samosan and Samoilenko are supported by the Newly Independent States Visitor's Program, a supplement to the NSF core grant to the NHMFL.

Odd-halves quadrupole nuclei represent great challenges and opportunities. To spectrally resolve chemically unique sites, many approaches have been developed to defeat second order broadening of the central transition due to the similar magnitude of the quadrupolar and Zeeman interactions. Higher fields directly reduce this broadening effect, as shown by many studies including recent experiments up to 25 T as described in the Fall 2000 *NHMFL Reports*. In this work, Zhehong Gan collaborated with Dominique Massiot from CNRS in Orleans, France to study aluminum sites in ${}^9\text{Al}_2\text{O}_3 + {}^2\text{B}_2\text{O}_3$. Four aluminum sites are much better resolved at 25 T than even at 19.6 T in magic angle spinning spectra. There are additional ways to enhance these quadrupolar spectra. One very successful approach for nuclei with small or modest quadrupole couplings involves multiple quantum magic angle spinning (MQMAS). A

recently developed and high sensitivity approach correlates the satellite transitions in two-dimensional MAS spectra (STMAS).¹ Now, an approach originally developed by Samosan, Lippmaa, and Pines² involving rotation about two octahedral axes simultaneously has been implemented at the NHMFL through Ago Samosan. Such a technology

operating in high field magnets has the potential to achieve very high resolution spectra even of nuclei with very large quadrupole interactions. The ${}^{17}\text{O}$ DOR (Double Rotation Spectroscopy) spectrum of KTP in Fig. 1 demonstrates the high spectral resolution from the DOR and the high field that resolves eight Ti-O-P sites in a chemical shift range less than 10 ppm.

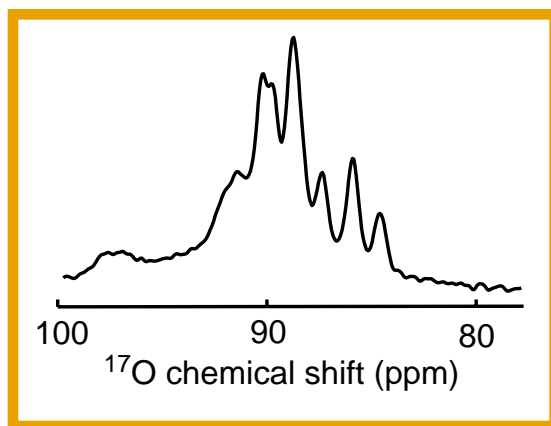


Figure 1. DOR (1400 Hz) spectrum of ${}^{17}\text{O}$ -enriched KTP at 16.9 T. Sample courtesy from Ray Dupree, University of Warwick/UK.

Imaging with NMR in the solid state suffers from a variety of problems, but one of the biggest problems is that linewidths are very broad. Efforts to image solids using MAS and synchronized acquisition has been demonstrated in several laboratories. Another approach to this problem is to use much larger field gradients than is normally used. A way to achieve this is to take advantage of the stray field of an NMR magnet.³ In a 19.6 T magnet approximately 20 cm below the center of the field is

a gradient of 75 T/m at a field strength of 11.7 T. This is equivalent to more than 3 kHz in ${}^1\text{H}$ frequency per micron giving rise to the potential for excellent spatial resolution even though resonances may be very broad. While it is not possible to pulse such gradients, it is possible to move the sample with respect to the gradient. In Fig. 2, we show one

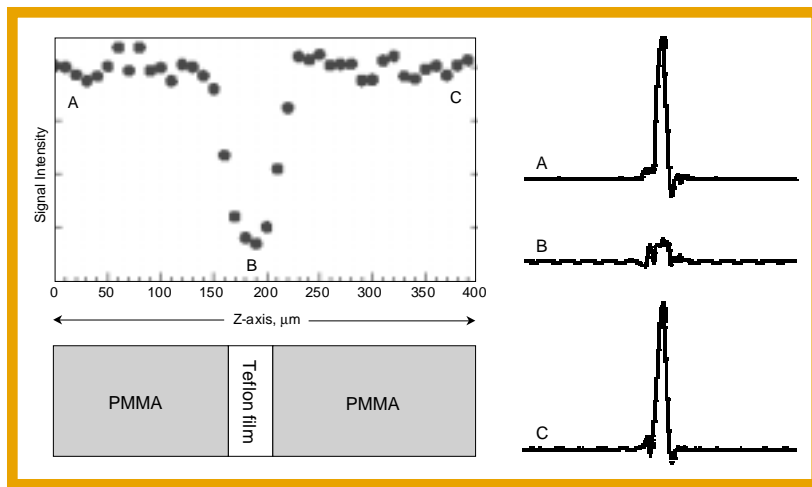


Figure 2. (left) 1D proton image of PMMA phantom with 39 μm Teflon film; (right) ^1H spectra from points A, B, and C in the image.

dimensional resolution of approximately 20 μm . Because the very large field gradients can dominate substantial magnetic susceptibility effects, it is possible to image even conducting samples.

The NHMFL is pleased to make these unique capabilities available to both national and international user communities. The DOR capability is available at a variety of superconducting fields up to 16.9 T and in resistive magnets up to 25 T. STRAFI is available today at 19.6 T, but the program has interests in adapting this technology to the resistive magnets. Those who are interested in using DOR should contact Zhehong Gan (gan@magnet.fsu.edu) and those interested in using STRAFI should contact Riqiang Fu (rfu@magnet.fsu.edu). For information on a wide range of other capabilities, please visit our Web site at <http://nmr.magnet.fsu.edu/>.

- ¹ Gan, Z., *J. Am. Chem. Soc.*, **122**, 3243, (2000).
- ² Samosan, *et al.*, *Mol. Phys.*, **65**, 1013, (1988).
- ³ Samoilenko, *et al.*, *JETP Lett*, (1988).

Structure and Regulation of the Diphtheria Toxin Repressor

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 P.D. Twigg, Florida State University, Biophysics
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We are investigating the structure and regulation of the diphtheria toxin repressor protein (DtxR), which is responsible for controlling the expression of the diphtheria toxin protein (Dtx), the protein that is the causative agent for the devastating systemic effects seen in diphtheria. There is significant interest in understanding how DtxR regulates the expression of Dtx because the DtxR protein might provide a unique target for the design of novel drugs that can be used to treat diphtheria. While diphtheria is not a significant health threat to the United States, diphtheria is still a debilitating disease found at epidemic levels in other parts of the world. Furthermore, the DtxR protein is the best characterized member of a family of related proteins that regulate toxin protein synthesis associated with other Gram-positive bacterial diseases including tuberculosis, syphilis, leprosy, and periodontal disease. A better understanding of how DtxR regulates toxin synthesis might provide insights

into the molecular basis for these more serious health threats.

Repressor proteins work by binding to sites in genes called promoters. The repressor prevents gene expression by sterically blocking recognition of the promoter site by the translational machinery in the cell. From microbiology experiments performed in other labs, it was known that DtxR activity was triggered by binding ferrous iron (Fe^{2+}), and DtxR was subsequently found to also regulate expression of siderophores, proteins that are required for iron uptake. Biochemical experiments showed that DtxR could not bind to the promoter site in the absence of Fe^{2+} , and that DtxR dimerized and bound tightly in a sequence-specific manner to the promoter for the diphtheria toxin gene in the presence of Fe^{2+} . Therefore, an initial working model for DtxR regulation involved a transition between monomer and dimer that was triggered by metal binding.¹

Structural studies performed in the labs of Dagmar Ringe and Wim Hol showed that this model was conceptually correct, but introduced a few unanticipated twists to the DtxR story.²⁻⁵ First, crystal structures of the apo- and metal bound-forms showed that DtxR formed nearly identical dimers in both states. Metal binding effected a small (3°) shift in the position of the two DNA binding helices. This minor structural difference contrasted strongly with the differential DNA binding ability mentioned above. Second, each DtxR monomer bound two equivalents of metal ions. This finding contradicted previous ligand-binding studies that indicated a single metal binding site per monomer. Third, DtxR bound to DNA as a dimer of dimers, with no apparent interaction between the dimers. Fourth, DtxR contains 226 amino acid residues per monomer, yet only the first ~140 amino acid residues were consistently observed in any of the crystal structures. These residues provided for the DNA and metal ion binding sites and the dimerization interface. The C-terminal ~86 amino acids were poorly characterized in the crystal structures, and its role in DtxR function was unknown. Furthermore, there was little amino acid sequence homology between this domain and any known protein. This precluded a prediction for the structure and function of the C-terminal domain and suggested that this domain may represent a unique, novel protein fold.

Because the C-terminal domain was poorly characterized by crystallography, we used high resolution NMR spectroscopy to determine the structure of this domain in solution. Our approach was to uniformly enrich the protein in ^{13}C and ^{15}N and then use a series of three dimensional heteronuclear experiments to obtain the complete sequence-specific assignments of every carbon, nitrogen, and proton in this domain.⁶ We then used these chemical shift assignments to interpret a series of multidimensional NMR spectra used to collect structural restraints. These restraints, which consisted of an extensive set of interproton distance restraints



Figure 1. Structure of SH3 domain in DtxR.

(from NOESY experiments), backbone torsion angles (from HN-H α scalar coupling constants), and the location of hydrogen bonds (from measurements of amide hydrogen exchange rates), were used to calculate a three dimensional

structure using a standard simulated annealing protocol.⁷ The C-terminal domain of DtxR consisted of a five-stranded β -barrel with two helices, Fig. 1. This domain is connected to the N-terminal domain by a flexible linker.

The structure determined for the C-terminal domain of DtxR is very familiar to structural biologists—it resembles that of SH3 domains. SH3 domains are small protein domains, or modules, typically found in proteins involved in signal transduction in eucaryotes. This structural similarity was surprising because the amino acid sequence of the DtxR SH3 domain is unrelated to that found in eucaryotic SH3 domains, and because SH3 domains had previously been identified only in eucaryotic organisms, yet the DtxR is a procaryotic, or bacterial, protein. In eucaryotes, SH3 domains bind to proline-rich segments of proteins, with high affinity ligands having a consensus sequence of Arg-X-Pro-Pro- ϕ -Pro, where X is any amino acid and ϕ is an amino acid with a hydrophobic sidechain. The high number of proline residues forces these segments to adopt a common structure, known as a polyproline type II (PPII) helix.⁸ In eucaryotes, SH3 domains can bind to PPII helices in an inter- or intramolecular manner. Intermolecular binding is involved in assembling multi-protein complexes and in protein-protein interactions involved in many biochemical pathways. Intramolecular SH3 domain – PPII binding functions to regulate protein activity. What was an SH3 domain doing in this procaryotic repressor protein? We identified a proline-rich region in DtxR (residues 125-135) that resembled the consensus high affinity sequences bound by eucaryotic SH3 domains, and demonstrated that the SH3 domain of DtxR bound to peptides containing this sequence, with a K_D of $\sim 2 \mu\text{M}$.⁷ These adopt a PPII helical conformation, and help stabilize the dimer interface in DtxR. We propose that binding of this Pro-rich region by the SH3 domain plays a role in regulating the activity of DtxR in the absence of metal ions by shifting the position of the monomer \leftrightarrow dimer equilibrium towards the monomer. This finding represents the first identification of an SH3 domain in regulating transcription and is the first example of intramolecular ligand binding in transcriptional regulation.

We are currently focusing on identifying how the DtxR SH3 domain recognizes and binds Pro-rich peptides. We are using isothermal titration calorimetry coupled with site-directed mutagenesis to determine accurate binding energetics and to define which interactions are crucial for ligand binding. We are also using NMR spectroscopy to determine the three dimensional structure of a complex between the DtxR SH3 domain and a peptide corresponding to the proline-rich region. It will be very interesting to compare PPII helix binding by the procaryotic SH3 domain with binding by eucaryotic SH3 domains because the amino acid sequences in the peptide binding sites are completely different. Knowledge of the chemistry involved in SH3 domain / ligand interactions for both eucaryotic and procaryotic domains may guide the development of novel small molecule compounds that modulate repressor activity,

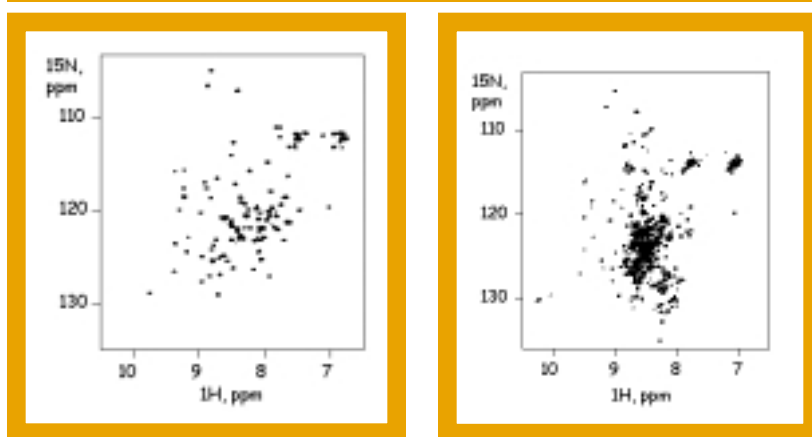


Figure 2. Two-dimensional ^1H , ^{15}N correlation spectra collected on full-length DtxR at 30 °C (left) and 4 °C (right).

signal transduction, cytoskeletal rearrangements, and other biological processes.

We are complementing our studies of the DtxR SH3 domain with structural and biophysical studies of full-length DtxR. From an NMR point of view, this is an exciting project as the protein is quite large (dimer of 226 residue monomers, molecular weight ~ 52 kDa) and represents a substantial challenge to current NMR methodology. Fig. 2A shows a 2D ^1H , ^{15}N correlation (HSQC) spectrum of DtxR in solution. This spectrum provides correlations between the amide hydrogen and nitrogen for every amino acid in DtxR (except Pro residues, which don't contain an HN), and we expect greater than 220 resonances in this simple spectrum. Clearly, we observe substantially fewer resonances. In fact, the resonances that are observed correspond to amino acids in the SH3 domain—none of the signals expected from the amino terminal 140 amino acid residues are observed. We determined that the signals from the amino terminal domain were undergoing conformational exchange on the intermediate chemical shift time scale, leading to extensive line broadening. By lowering the temperature to 4 °C, we observe numerous resonances that indicate regions of ordered and disordered structure. Circular dichroism showed a native amount of secondary structure, while fluorescent dye-binding assays showed the protein was in a non-native conformation. In other words, the N-terminal domain adopts an ensemble of partially ordered, rapidly interconverting structures in solution in the absence of metal ions, similar to the “molten-globule” structure seen as intermediates in protein folding studies. Furthermore, we observe large changes in the HSQC spectra of DtxR in the presence of (diamagnetic) Cd^{2+} , consistent with a metal ion-binding induced ordering in the three dimensional structure of DtxR.⁹ Ligand-induced folding transitions have been identified in numerous DNA-binding proteins, where they provide an additional level of regulation on repressor activity.¹⁰ The conformational flexibility may also be important when

the repressor binds to several different promoter sites, as in DtxR. Finally, a ligand-induced folding transition provides a better explanation for the differential DNA-binding by apo- versus metal-bound DtxR.

Ironically, X-ray crystallography “sees” the N-terminal domain but not the SH3 domain, whereas the SH3 domain, but not the N-terminal domain, is “seen” by NMR. This is a prime example of how information from different structural biology techniques complement each other. We are working to define the regions of ordered structure in apoDtxR in solution, and to understand how ligand binding changes the structure. These

studies will combine NMR spectroscopy with FT-ICR, again, highlighting the importance of complementary approaches to structural problems in biology.

Driving a car would be extremely dangerous without gas pedals and brakes to control the cars speed. So it is with proteins, whose activity can be increased or decreased in response to environmental conditions. Our studies on DtxR have revealed that several regulatory mechanisms (metal-ion binding, dimerization, folding, and intramolecular peptide binding) converge on this single protein. Understanding how these mechanisms combine to provide the biologically effective regulation will have relevance for protein regulation, in general.

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- ² Qiu, X., Verlinde, C.L.M.J., Zhang, S., Schmitt, M. P., Holmes, R.K., and Hol, W. G. J. (1995) *Structure* **3**, 87-100.
- ³ Schiering, N., Tao, X., Zeng, H., Murphy, J.R., Petsko, G.A., and Ringe, D. (1995) *Proc. Natl. Acad. Sci. USA* **92**, 9843-9850.
- ⁴ White, A., Ding, X., Spek, J.C.V., Murphy, J.R., and Ringe, D. (1998) *Nature* **394**, 502-506.
- ⁵ Pohl, E., Holmes, R. K., and Hol, W.G.J. (1998) *J. Biol. Chem.* **273**, 22420-22427.
- ⁶ Twigg, P.D., Wylie, G.P., Wang, G., Murphy, J.R., Caspar, D.L.D., and Logan, T.M. (1999) *J. Biomol. NMR* **13**, 197-198.
- ⁷ Wang, G., Wylie, G.P., Twigg, P.D., Caspar, D.L.D., Murphy, J.R., and Logan, T.M. (1999) *Proc. Natl. Acad. Sci., USA* **96**, 6119-6124.
- ⁸ Yu, H., Chen, J.K., Feng, S., Dalgarno, D.C., Brauer, A.W., and Schreiber, S.L. (1994) *Cell* **76**, 933-945.
- ⁹ Twigg, P.D., Guerrero, L., Parthasarathy, G., Logan, T.M., and Caspar, D.L.D. (2001). “A disordered-to-ordered structural transition is involved in regulating repressor activity in the diphtheria toxin repressor”, *in the press, Proc. Natl. Acad. Sci. USA*.
- ¹⁰ Spolar, R.S., and Record, M.T. (1994) *Science* **263**, 777-784.

Open House 2001 - Visitors, Faculty, and Staff Enjoy Science Together

On March 3, the NHMFL held its 7th Annual Open House. Over 40 different research and engineering groups in the laboratory participated in demonstrations and hands-on activities, as well as 14 science and education organizations from the community. This year's theme, "Supporting Science, Education, and Our Community," was emphasized through the *Science in My Community Contest*. The goal of the contest was to encourage students, classes, families, and community groups to look beyond the laboratory and explore science at work in the many communities around them: classrooms, schools, homes, neighborhoods, and the world. All participants were recognized for their contributions with a display of their projects and certificates of participation. First Place, Second Place, and Honorable Mention Prizes were awarded in several categories and included multimedia resources such as: QX3 microscopes, classroom libraries, and curriculum resources.

The overall grand prize winner was Ms. Petty's Wesson Elementary School class, for their poster and video entry "Photosynthesis in Our Community." The overall runner-ups were Ms. Holden's Quincy Educational Academy high school class, for their poster, display, book, and brochures entry "Obesity in the African-American Community." During the award ceremony, NHMFL Director Jack Crow reflected on the high level of anticipation that surrounds Open House year after year. He noted that some people drove great distances to pick up their awards, and he was impressed with a couple from Jacksonville who had traveled the night before and spent the night in a hotel, just so they could be at Open House when the doors opened. They were one of the last groups to leave.

Highlights from the many scientists and staff who participated in the Open House included: a 3D show featuring an Environmental Scanning Electron Microscope, a superconducting maglev train showcasing the frontiers of transportation, a penny press and "bending nails" activity that demonstrated the power of pressure, moon rocks brought to Tallahassee from the Kennedy Space Center, and a demonstration of the effects of changing atmospheric pressures that involved marshmallows in a vacuum chamber (during the activity, the marshmallows, which had dots painted on them, expanded to look like eyeballs, then collapsed to smaller-than-original size).

Community participation by the laboratory's *Community Science and Education Partners* included the St. Marks Wildlife Refuge, Academic Resource Center (ARC), Girl Scouts, Tallahassee Museum of History and Natural Science, United States Geological Survey, Joe Budd Aquatic Education Center, Leon County Public Library, Birdsong Nature Sanctuary, and many others.



"Obesity in the African-American Community"

Overall Runner-up
Quincy Educational Academy
Ms. Holden's Class

Dr. Crow Presents Awards

"Ships, Science and Surfboards"
2nd Place K-2, Individual
Home School



Sylvie Fuzier, a graduate research assistant with the NHMFL Magnet, Science, and Technology (MS&T) Group, helped with a cryogenics



demonstration, where balloons of gas were placed in liquid nitrogen to cool them down. Nitrogen-filled balloons did not experience any changes because it was not cold enough; oxygen-filled balloons filled with blue liquid because oxygen is blue, and carbon-dioxide-filled balloons filled with white powder, i.e., became solid "dry ice." Fuzier was surprised by the excitement and interest expressed by the children and adults who asked many questions.



Center for Research and Learning (CIRL) graduate research assistant, Amudha Jayaraj, was kept busy with the many hands-on, educational activities her group had to offer, including refrigerator magnet-making, a model-sized neighborhood with a magnet maze, and optics.



Robert Hudgins, a postdoctoral research associate with the Center for Interdisciplinary Magnetic Resonance-Ion Cyclotron Resonance (CIMAR-ICR) demonstrated different vacuum technologies with hands-on hardware.



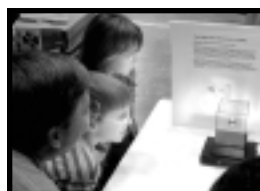
The FSU Sensory Research Institute (SRI), located in the NHMFL, displayed a demonstration on the operation of a dog olfactometer that middle school students, Evan McClellan and Bradley Troast, helped build as a part of the NHMFL/Leon County-ARC Middle School Mentorship Program. The display featured the current research study using dogs to detect disease.



Bruce Brandt, Director of DC Field Facilities, helped with the “smashing pennies” demonstration that allows visitors to work a hydraulic press in the high pressure lab. He enjoyed observing the different experimental styles: the goal-oriented watched the dial and stopped on the line, the process-oriented pumped away until someone said “stop,” the people-oriented played to their group, the plucky little ones could barely work the pump, but gave it their all, the shy hung back until everyone else in their group had tried it out, and the fathers and mothers were a little embarrassed to be interested in a phenomenon that attracted mostly children!



The Condensed Matter Science Program was pleased that their group’s small, hands-on demonstrations, intended to be “fun,” were such a hit with children.



Education Program Extends Outreach and Prepares for Busy Summer

The NHMFL's Center for Integrating Research & Learning continues its work with teachers and students through classroom and community outreach, teacher workshops, and new partnerships with schools and districts. The NHMFL is currently hosting 23 middle school students through a mentorship program that the Center has coordinated for the last several years. As an active partner with a local elementary magnet school for science and mathematics, the Center provides teacher in-service, serves on its planning committee, and supports teachers through the Research Experiences for Teachers (RET) program. The Center recently received another supplemental award to support the RET program in summer 2001. In an effort to comply with Florida's science benchmarks, the Center anticipates taking an active role in assisting schools and school districts as they provide support for teachers. It is currently building new partnerships with neighboring counties to assist in their quest to raise test scores and address mandated science testing for fifth, eighth, and tenth graders.

An RET workshop was held as part of the spring Materials Research Society (MRS) meeting in San Francisco, California. The symposium entitled, "Impacting Society Through Materials Science and Engineering Education," brought together program leaders from around the country. Former CIRL Director, Sam Spiegel, opened the program with a presentation entitled, "Using Science Education to Impact Important Societal Issues." Other representatives from the University of Wisconsin, Northwestern University, Harvard University, and Columbia University presented examples of their programs and a preliminary look at the assessment of the impact of the program. Round table discussions were held and panel recommendations were summarized at the end of the symposium. A report will be drafted by the MRS and made available in the near future.

Science, Tobacco & You Best Practices 2001 occurred in three locations across Florida on April 26, 2001. The seminar, a live satellite broadcast and awards ceremony,

was an opportunity for 300 teachers and 30 students to showcase the curriculum resource *Science, Tobacco & You* and how they have adapted it to meet their needs. Connecticut and Illinois teachers have been participating in *Science, Tobacco & You* workshops, and the program continues to expand to other states as well.

Several students who participated in Summer 2000 Research Experiences for Undergraduates (REU) have

had their research reports accepted for publication. Working with mentors Donovan Hall, Eric Palm, and Stan Tozer in Tallahassee, students Eliza Miller-Ricci, Lydia Peabody, and Charis Quay are listed as co-authors for an article published in *Physical Review*. James Maloney, under the mentorship of Mark Meisel at the University of Florida, published his work under the title "Low Temperature Capacitance Measurements of a Novel Low-Dimensional System" in the *Journal of Undergraduate Research*.

Once again, the Center is in the throes of preparing for the Research Experiences for Undergraduates (REU) program through which the NHMFL will host 17 students, 13 at the Tallahassee site, three at UF, and one at LANL; and the Research Experiences for Teachers (RET) program, which will be working with 16 teachers. The Center is looking forward to a busy and rewarding spring and summer.



Advanced Magnetic Resonance Imaging and Spectroscopy (AMRIS) Facility Progress and Research Report #6, April 2001

by Steve Blackband, Associate Professor, UF Neuroscience

AMRIS Progress, April 2001

1. 750 MHz magnet for NMR/MRI. In the last report, we described that over a few hours the magnet homogeneity falls off significantly due to coupling between the wide bore shims and the cryoshims when the wide bore shims are switched over to the narrow bore shims, thus limiting high resolution spectroscopy studies. To circumvent this issue, Bruker supplied a second shim set power supply and control boards so that the wide bore shims may be left powered on when the narrow bore shims are used. This appears to have cured the drift problem and the instrument has now been accepted. Shimming, however, is clearly more difficult at this higher field and there will be a considerable learning curve to get the most out of the machine.

Probe development will be a major issue for this instrument. To this end, we recently hired Sam Grant from Chicago, a previous student of Andy Webb's and an outside user of the 600 MHz wide bore at the NHMFL, into a postdoctoral position. Sam will be developing rf probes on the 750 MHz, starting with a range of microcoils.

2. 11.7 T/40 cm magnet for MRI. As reported in the last update, the 11.7 T cryogenics leaked severely leading to an ice build up in the magnet. Using a specially ordered scope, the ice could be viewed at least on the top plate in the magnet. A considerable amount of effort was expended by Magnex to try and clear the ice using a heated nitrogen gas jet. This ultimately failed, however, and after meeting with Magnex shortly after Christmas, it was decided that there was no option other than to warm up the entire magnet and try to clear out the water build up. Since this process had to be performed, the opportunity was also taken to completely overhaul the cryogenics. This was performed by Tim Carney of Magnex who has successfully installed a 11.7 T/33 cm instrument at the NIH (of the same design as our 11.7 T/40 cm). Additionally, the rf roof over the magnet is being raised 3 feet to make filling easier and safer. There was also some concern voiced over the safety of the magnet system, but meetings and discussions between Magnex and Steve Van Sciver of the NHMFL in Tallahassee have alleviated this issue—thanks Steve.

At this point in time, the magnet is at room temperature and gas is being blown clear through the water—the outgoing gas is still 20% humid so it is not at all clear how long this process will take. I have given up extrapolating dates the magnet will be up and running so don't ask!

In the meantime, Alan Koretsky and Alonso Silva generously let us travel to the NIH so that we could use their 11.7 T and time to test new volume coils that Barbara Beck has been developing. Many thanks for their spirit of

collaboration. Further trips may take place if the magnet is significantly delayed further.

Two new staff members have been added to AMRIS to help replace Ben Inglis and to support new users on our now larger instrument base. Gary Blaskowski has a physics background and is being trained to maintain and run the 4.7 T/33 cm and 11.7 T/40 cm instruments. Additionally, Xeve Silver has a biological background and has been hired part time to help facilitate animal experiments and assist users.

3. We are very pleased to announce that our site visit last October for our application to the NIH to become a National Resource (a P41 grant) went extremely well. We are expecting funding and are awaiting the receipt of the grant award starting May or June 2001. This was a large collaborative effort, including co-workers at the NHMFL and several outside users. Many many thanks again to all involved.

Partly as a consequence of the need to direct the Resource, and our original plan that the AMRIS director be a rotating two-year term, I will be stepping down as AMRIS director in June. The next newsletter will be my last and I will be handing over the reigns to Art Edison—he will have plenty to do!

The following research report briefly describes the development of phased array rf coils on our 4.7 T instrument.

AMRIS Research Report #6

Phased Array Coils at 4.7 T

B.L. Beck, UF McKnight Brain Institute, NHMFL
B.A. Inglis, UF McKnight Brain Institute, NHMFL
S.J. Blackband, UF Department of Neuroscience, UF McKnight Brain Institute, NHMFL

Phased array technology was first introduced to the MR world in 1990¹ and offered the high signal-to-noise of smaller surface coils over large fields-of-view (FOV). Phased array volume coils² were introduced shortly after the surface coil arrays and provided enhanced SNR near the surface of the volume without compromising SNR at the center. Phased array technology has since become a standard in clinical MR imaging, with phased array coils available for head, neck, spine, wrist, hand, knee, foot, shoulder, breast, pelvis, and more. Phased array technology is just beginning to move into the animal research realm and the manufacturers of small animal research systems are now making some of the necessary phased array hardware available. Bruker Instruments Ltd. (Billerica,

USA) has recently provided the multiple radio frequency (rf) channels on our 4.7 T/33cm spectrometer console. We have developed the rest of the equipment required for phased array operation, namely the rf array coil, low impedance preamplifiers, excitation coil, and image combination.

A receive-only 4-channel phased array coil (Fig. 1) for imaging cat spines was built on an acrylic half cylinder 5 1/2" in diameter. Each loop in the array was 4 cm by 5 cm. Coil isolations were >20 dB on all channels partly by using low input impedance preamps (1) mounted on the coil. It was necessary to provide our own preamplifiers because the magnet system manufacturer offers preamps with 50 ohm inputs on its phased array system. Preamplifiers were purchased from Advanced Receiver Research (Burlington, CT) and modified to achieve an input impedance of ~4 ohms real, noise figure of 0.6 dB, and gain of 21 dB.

The array was surrounded by a large half-saddle transmit coil 19 cm in length. A loaded isolation between the transmit coil and the receive array of >30 dB was achieved. The coils were loaded with a large cylindrical phantom with loading equivalent to a cat, and spin echo images of the phantom were acquired. A composite image from the array coil was created by applying the sum-of-squares technique to the magnitude images of each array element. Fig. 2 shows

the images that were simultaneously acquired from the individual channels of the array, along with the composite sum-of-squares image.

In this work we have provided the above pieces to develop a phased array coil for imaging cat spinal cords on a 4.7 T Bruker Avance, and have demonstrated the feasibility of phased array coils on animal research systems. To our knowledge, this is the first phased array coil constructed for an animal system and also the highest frequency phased array coil yet constructed. We are presently exploring similar developments at even higher field strengths (our 11.7 T/40 cm also has phased array capability). This coil is now being evaluated in animal studies and will be presented at the ISMRM this year and submitted for publication.

Acknowledgements. This work was supported by the University of Florida McKnight Brain Institute, Gainesville, FL, and the NHMFL. The authors thank Mark Mattingly of Bruker Medical for his support in hardware and software installation.

¹ Roemer, P.B., *et al.*, *Magn. Reson. Med.* 16, 192-225 (1990).

² Hayes, C.E., *et al.*, *Magn. Reson. Med.* 18, 309-319 (1991).

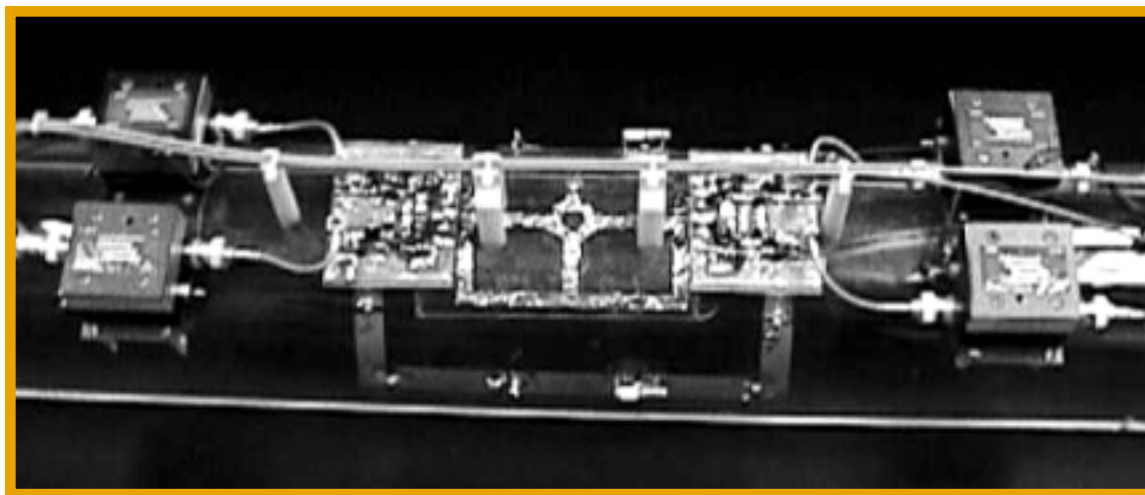


Figure 1. The phased array coil consisting of the central four receiver coils and the larger transmit coil and associated hardware. Note the two pairs of preamps on the far left and right.

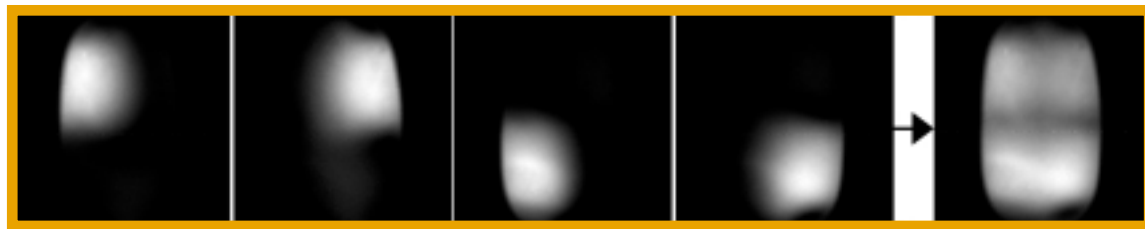
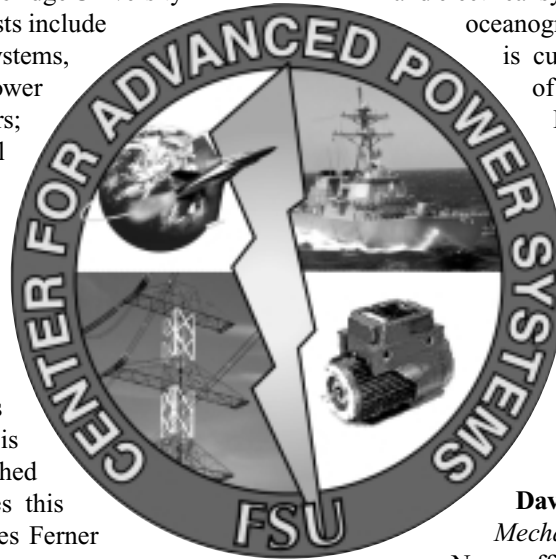


Figure 2. Four images from the four coils (left) summed together to make a composite image (right).

Center for Advanced Power Systems Faculty Grows

Peter G. McLaren, Director. Presently, Dr. McLaren is serving in a consulting capacity to CAPS, but in June he will assume new duties as the full-time director. He is from the University of Manitoba and was previously a professor of engineering at Cambridge University in England. His research interests include simulation of electrical power systems, off-line and real time; the power applications of superconductors; signal processing; and optical transducers for power system instrumentation and control. Not only does he come from a strong academic background, but McLaren also has extensive experience with industry research in power system development. He has advised many students and is a frequent lecturer and published author. When McLaren arrives this summer, Interim Director James Ferner will become CAPS Deputy Director.

Michael Steurer, Assistant in Research. Dr. Steurer recently received his Ph.D. from the Federal Institute of Technology in Zurich. His research interests are power switching systems, fault current limiters, and power systems.



Cyril F. Krolick, Associate Director. Dr. Krolick brings extensive experience in naval ship systems with thirty years logged in conjunction with the Naval Service Warfare Center and five years as a consultant in machinery and electrical systems for naval, commercial, and oceanographic applications. Dr. Krolick is currently Chief Operating Officer of Syntek, a naval consulting firm. He received his Ph.D. in Nuclear Engineering and Electrical Engineering from the University of Maryland in College Park. Dr. Krolick will work part-time for CAPS and continue to reside in Washington, D.C., where he coordinates industrial and program activities with the Office of Naval Research.

David A. Cartes, Assistant Professor, Mechanical Engineering. A former Navy officer with experience in nuclear propulsion and shipbuilding, Dr. Cartes's alma mater is Dartmouth College. His research has focused on active acoustic and electromagnetic noise cancellation and his work with CAPS will specialize in controls.

CENTER FOR ADVANCED POWER SYSTEMS FLORIDA STATE UNIVERSITY

Positions Available

Semester Sabbaticals: We have a limited number of positions for semester sabbaticals for faculty who are interested in power systems research, curriculum development, and limited teaching in our new power systems program.

Postdoctoral Positions: A number of postdoctoral opportunities in power systems are available.

Faculty Positions: Several tenure-track faculty positions are available in the EE and ME departments for individuals with interests in power systems and related technologies.

For more information on these opportunities, please contact James Ferner, Interim Director, Center for Advanced Power Systems, Florida State University, Tallahassee, FL 32306-2740, 850-644-9630, ferner@caps.fsu.edu.

People in the News



Timothy A. Cross, NHMFL Nuclear Magnetic Resonance (NMR) Program Director and professor of chemistry, was awarded the FSU Distinguished Professor Award. This award, recognizing outstanding

achievements in research and creative activity, was one of three given university-wide this year. Cross's research interests include understanding how biological macromolecules, specifically membrane proteins, carry out their functions. His work in the arenas of structural biology and structural genomics results in the structural and dynamic characterization of membrane proteins. His group also publishes on the development of solid state NMR methodology for macromolecular studies and on the development of high field NMR technology and applications.

Julie Gallegos has joined the NHMFL in Los Alamos as their Program Administrator. In addition to handling budget issues, she is working with Alex Lacerda organizing the Physical Phenomena in High Magnetic Fields -IV conference to be held in Santa Fe on October 20-25, 2001.



Ron Hills, a sophomore biochemistry major at FSU, has received a prestigious Goldwater Scholarship. Since his second semester at FSU, Ron has been working on the structure of muscle regulatory protein, troponin, using

spin labeling approaches in Peter Fajer's lab at the NHMFL. Established in 1986 by Congress, the Barry M. Goldwater Scholarship and Excellence in Education Foundation seeks to encourage outstanding students in the fields of mathematics, the natural sciences, and engineering. Hills has also received two NSF and two American Cancer Society fellowships.

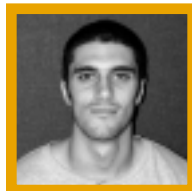
Kee Hoon Kim will be joining the NHMFL from Seoul National University as a LANL Director's funded postdoc. Kim will be working with Greg Boebinger and Marcelo Jaime on experiments searching for quantum critical points in correlated systems.



Asa Hopkins, who interned with Stan Tozer at the NHMFL before and after his freshman year at Haverford College, has been awarded an NSF Graduate Fellowship. A two-time, first-team Academic All-America selection and 1999 Goldwater Scholar, Hopkins will be attending the California Institute of Technology (Caltech) Ph.D. program in physics after working at LANL for a year. Hopkins says, "I really enjoyed working at the magnet lab. My work there was instrumental in my receiving a Goldwater Scholarship, which in turn has helped me in my graduate school search, and in securing a job for next year."

Christine A. Hughey, FSU Ph.D. candidate and graduate research assistant in the NHMFL ICR Program, was awarded the Kenan Award by Union Carbide (now Dow Chemical) at an award symposium held on April 9-11. The top 35

analytical chemistry departments in the United States each nominated three graduate analytical chemistry students. Of those 105 promising students, 10 were chosen to receive the award. Each award-winning student gave a 20-minute talk about his or her graduate research and interacted with scientists in industry. Hughey's graduate research is about the "Resolution and Chemical Identification of Petrochemicals by Use of Electrospray Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FT-ICRMS)."



Clement Rouviere, a junior in the FSU Department of Nutrition, Food and Exercise Sciences, has received a Eunice Grady Endowed Scholarship given by the FSU College of Human Sciences. Rouviere is working in Piotr Fajer's lab at the NHMFL on a project funded by the Muscular Dystrophy Foundation to solve the structure of troponin, protein, which activates muscle contraction. Rouviere has also received an NSF research fellowship and will be continuing his education at the lab this summer.

FSU Research Awards



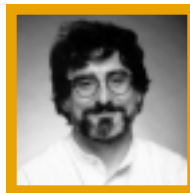
A multidisciplinary team of FSU researchers are the recipients of up to one million dollars to establish the FSU Research Foundation's third Center of Excellence. This award will establish the Center in Earth Surface Processes, which will research applications of advanced computing in studies of flow and transport in hydrological and geomorphic systems. **Yang Wang**, a professor of geochemistry, who works in the Isotope Geochemistry Laboratory located at the NHMFL, is a core participant in the award-winning proposal. Other investigators include: PI, *David Furbish*, *Mark Scmееckle*, and *Yousuff Hussaini*. Wang is currently researching coastal wetland formation and its significance to carbon sequestration; the source and fate of dissolved organic carbon and phosphorous in Florida Everglades; the factors and processes controlling carbon emission from soils; and the paleodiet and paleoenvironment of fossil mammals in China.

In addition, two NHMFL-affiliated research teams received Program Enhancement Grants (PEG) of approximately \$100,000 each.

James C. Smith, FSU professor of psychology and scientific advisory board member for the Sensory Research Institute located at the NHMFL, and **Thomas Houpt**, professor of biological science at FSU, are researching the project,

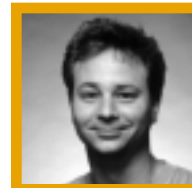


"Behavioral and Neural Effects of High Strength Static Magnetic Fields" in which they use the magnets at the NHMFL to aid in their experiments. Smith, a 1992-93 Robert O. Lawton Distinguished Professor, is currently researching the sensory capabilities of rats in detecting high intensity magnetic fields of 4 T and higher.



Piotr Fajer, professor of biological science at FSU and member of the NHMFL Center for Interdisciplinary Magnetic Resonance (CIMAR)/Electron Magnetic Resonance Group, along with **Timothy Logan**, FSU professor of Chemistry and

member of the NHMFL CIMAR/ Nuclear Magnetic Resonance Group, and FSU chemists *Michael Blaber*, *Edwin Hilinski*, and *Albert Stiegman* are researching the project, "Program in Real-Time Electron Paramagnetic Resonance for the Life and Chemical



Sciences." Fajer, who received an FSU Teaching Award in 1998 and Developing Scholar Award in 1997, has research interests in protein structure and function, and electron paramagnetic resonance: time-resolved EPR spectroscopy and computational analysis. Logan, associate director for solution state spectroscopy, researches how protein structure and dynamics are related to biological function. One of his projects involved the development and characterization of triple-resonance microcoils for high resolution NMR spectroscopy in high field magnets.



The research staff at the NHMFL in **Los Alamos** has been awarded a LANL Laboratory Director's Research and Development grant to develop phase sensitive gigahertz techniques for use in pulsed magnetic field experiments.

Conference & Workshop Activity

Fifth MRS/ISTEC Joint Workshop on High Tc Superconductivity

June 24-27, 2001

Honolulu, Hawaii

The general theme of this workshop is Processing and Applications of High Tc Conductors, with a special focus on HTS Coated Conductors. The NHMFL is a partial sponsor, along with Oak Ridge National Laboratory, Los Alamos National Laboratory, Argonne National Laboratory, and the University of Wisconsin. ISTEC is a Japanese organization; MRS is the Materials Research Society.

24th International EPR Symposium

July 29-August 2, 2001

Denver, Colorado

Pre-Conference Registration Deadline: July 1, 2001

<http://www.du.edu/~seaton/eprsym.html>

<http://www.milestoneshows.com/rmcac/>

The 24th International EPR Symposium will be held in conjunction with the 43rd Annual Rocky Mountain Conference. About 150 people participate in the EPR Symposium each year, presenting over 100 papers. Approximately 1,000 people attend the Rocky Mountain Conference, which also includes an NMR Symposium and instrument exhibit.

The International EPR Symposium covers all aspects of EPR spectroscopy. This year there will be sessions emphasizing the wide range of frequencies at which EPR is now performed including, for example, *in vivo* experiments at 250 MHz and high field EPR. The NHMFL is helping to sponsor the high field sessions. There also will be a special session on industrial applications of EPR.

Fifth Latin American Workshop on Magnetism and Magnetic Materials and their Applications

September 3-7, 2001

San Carlos de Bariloche, Argentina

Pre-Conference Registration Deadline: June 30, 2001

<http://www.cab.cnea.gov.ar/calendario/law3m/>

This will be the first meeting of this workshop of the new millennium and the fifth of a series initiated in La Habana, Cuba in 1991; other workshops were held in Guanajuato, Mexico (1993), Merida, Venezuela (1995), and Sao Paulo, Brazil (1998). LAW3M is designed to bring together the Latin American community of scientists and engineers interested in recent developments in both fundamental and applied magnetism, on topics such as thin films, giant magnetoresistance and magnetoelectricity, nanocrystalline materials, superconducting oxides, and magneto-optics. The program will consist of invited and contributed papers, tutorial in nature, as well as reviews of recent work in specialized fields.



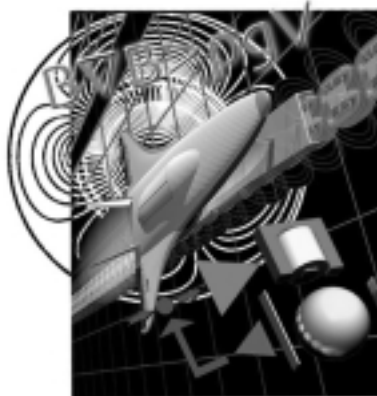
6th International Symposium on Magnetic Suspension Technology

October 7-11, 2001
Turin, Italy

Pre-Conference Registration Deadline: June 30, 2001
<http://www.lim.polito.it/ISMST6>

The 6th ISMST will be hosted by the Technical University of Turin with support from the NHMFL. The symposium will be held at the Centro Congressi with easy access to the railway station and bus stops to tour the city. This biannual meeting will cover a wide range of magnetic suspension topics, including magnetic bearings, electromagnetic launch, sensors, controls, related high- and low-temperature superconducting magnet technology, wind tunnel model suspension, and design and implementation practices. Industrial applications include magnetic bearings for high-speed rotating machinery, levitated trains, vibration isolation, pointing and control, and guiding systems. An exciting new area is materials processing and biological studies in low or zero gravity by magnetic suspension.

Conference co-chairs are Giancarlo Genta of the Technical University of Turin and NHMFL Deputy Director Hans Schneider-Muntau. Complete information is available on the conference Web site, but interested parties may also direct inquiries by e-mail to ismst6@magnet.fsu.edu (NHMFL in Tallahassee) or ismst6@polito.it (Politecnico di Torino). The abstract deadline is May 15, 2001.



Physical Phenomena at High Magnetic Fields (PPHMF-IV)

October 19-25, 2001
Santa Fe, New Mexico

Hotel Headquarters: Hilton and Radisson of Santa Fe
Pre-Conference Registration Deadline: June 1, 2001
<http://www.lanl.gov/mst/nhmfl/PPHMF4/>



This major international conference brings together experts to discuss recent advances in areas of science and applications in which high magnetic fields play an important role. Topics will include: semiconductors, magnetic materials, superconductivity, organic solids, the quantum Hall effect, chemical and biological systems, and the technological use of high magnetic fields. Initiated by the NHMFL in 1991, this conference is held every three years. The abstract deadline is June 1, 2001.

Applied Superconductivity Conference (ASC04)

October 4-8, 2004
Site: Jacksonville, Florida

This important international conference is held every two years and typically attracts approximately 1,800 participants. In September 2000, ASC00 was held in Virginia Beach, Virginia; in August 2002, ASC02 will be in Houston, Texas; and in October 2004, ASC04 comes to Jacksonville, Florida. For information, contact ASC04 Conference Chair Justin Schwartz in NHMFL's Magnet Science & Technology program, 850-644-0874, fax 850-644-0867; schwartz@magnet.fsu.edu.

J. Robert Schrieffer Anniversary Symposium

October 19, 2001

Sante Fe, NM

The NHMFL will be hosting a special one-day symposium in honor of its Chief Scientist, Robert Schrieffer, in recognition of his 70th birthday and his enormous contributions to condensed matter physics. The symposium will precede the Physical Phenomena at High Magnetic Fields IV conference that Dr. Schrieffer founded in 1991. The symposium will feature Nobel laureates and other distinguished scientists with a focus on the theory of high temperature superconductivity and magnetism in condensed matter systems. The program committee is being chaired by Steve Kivelson and consists of Nicholas Bonesteel, James Davenport, Ted Einstein, Douglas Scalapino, and John Wilkins. If you would like more information regarding this symposium, please contact Mary Layne via e-mail at layne@magnet.fsu.edu or visit the NHMFL Web site at <http://www.magnet.fsu.edu/>.



Multi-Institutional Project Focuses on Synthetic Metals by Bruce Brandt

Participants in a multinational cooperative project to study “Quantum Transport in Synthetic Metals” gathered at Seoul National University (SNU) on May 8-11 to discuss their progress to date. The project and conference were organized by Dr. Yung Woo Park, professor and Director of the Condensed Matter Research Institute at SNU. James Brooks’s group at the NHMFL has participated actively in the multinational project, sending some students to Seoul, and publishing papers on uniaxial stress investigations of the modification of superconductivity in low dimensional materials, thermopower measurements in very high magnetic fields, and the use of high field thermopower to investigate the high field state of an anomalous charge density wave state.

Professor Park’s group has visited the NHMFL regularly to use high magnetic fields to examine the roles of intra- and inter-fibrillar interactions in electrical conduction processes in doped polyacetylene. (The 2000 Nobel Prize in Chemistry recognized pioneering research on conducting polymers by Professors Heeger, MacDiarmid, and Shirakawa.) The Park group has shown that three-dimensional (anisotropic) weak localization theory, which is usually applied in the case of doped high-density polyacetylene at low magnetic field, is not appropriate to explain the high magnetic field ($H > 30$ T) dependence of the conductivity of the doped helical polyacetylene. They also suggest that the unusual features of the electrical conductivity of the disordered system formed by polyacetylene doped with FeCl₃ are due to a significant spatial inhomogeneity of the conduction band edge.

Other participants in the multinational cooperative project are Alan J. Heeger at UCSB; Hideki Shirakawa at U. of Tsukuba; S. Roth and Klaus von Klitzing at Max Planck Institute, Stuttgart; P. Bernier at U. Montpellier II; Alan Kaiser at Victoria U. in Wellington, New Zealand; and Robert Schrieffer, Zachary Fisk, and Jack Crow of the NHMFL.

This article was contributed by Bruce Brandt, who may be contacted for further information at brandt@magnet.fsu.edu.

Presenting the NHMFL's Newest Doctors

The laboratory is pleased to recognize its Class of 2000. During end-of-year annual reporting, we learned that the following outstanding young scientists received their doctoral degrees last year. They were advised by NHMFL faculty or users and participants in active research projects. Congratulations and best wishes as they pursue new endeavors.

Buhler, Charles, *Numerical Simulations of High T_c Superconductors*, Florida State University, Physics

Callihan, Dana E., *Structural Characterization of Peptide Fragments from the FK506 Binding Protein: Modeling the Earliest Events in Protein Folding*, Florida State University, Chemistry

Cothorn, John A., *Dynamics of Granular Media in a Magnetic Force Environment*, Florida State University, Physics

Denny, Jeffrey K., *Geometry of Proteins with Applications to Solid-State Nuclear Magnetic Resonance*, Florida State University, Mathematics

Huang, Wei, *A Comparative Study of the Melting and Crystallization Behavior for Metallocene and a Narrow Fraction of Ziegler-Natta Isotactic Polypropylene*, Florida State University, Chemical Engineering

Jackson, Damon, *Anisotropy in Magnetic and Transport Properties of $RTSb_3$* , Florida State University, Physics

Jung, Jung-Hoon, *Optical Studies of Charge/Orbital Ordering in Manganites*, Seoul National University, Physics

Kim, Do-Hyun, *Growth and Zeeman Spectroscopy of GaAs/AlGaAs Quantum Wire Arrays in Various Wire Widths*, Seoul National University, Physics

Kmety, Carmen R., *Phase Transitions in Molecule-Based Magnets: Neutron Diffraction, Magnetic and Specific Heat Studies*, The Ohio State University, Physics

Mertz, Laura, *Peptide Binding Studies of the C-Terminal Domain of Diphtheria Toxin Repressor Protein*, Florida State University, Chemistry

Munteanu, Florin M., *Magneto-Optical Experiments in GaAs/AlGaAs Heterostructures*, Northeastern University, Physics

Nam, Moon-Sun, *Magnetotransport in BEDT-TTF Salts*, University of Oxford, Physics

Ohmichi, Eiji, *Oriented Magnetic Field Effects in Quasi Two-Dimensional Superconductors*, Kyoto University, Physics

Pan, Wei, *Experimental Studies of the Even-Denominator Fractions in High Landau Levels*, Princeton University, Physics

Petrovic, Cedimir, *On the Absence of Magnetism in Quasi-2D Ternary Rare Earth Intermetallics*, Florida State University, Physics

Raghavan, Karthik, *Rapid Computational Methods for Velocimetry and Diffusion Measurements from Images Obtained Using Pulsed Field Gradient Techniques in Magnetic Resonance Imaging*, Florida State University, Chemical Engineering

Schrama, J.M., *Magneto-Optics of Quasi-Two-Dimensional Metals*, University of Oxford, Michaelmas, Physics

Stalcup, Thomas F., *Transport and Magnetic Properties of an Organic Superconductor*, Florida State University, Physics

Subramanyam, Pilla, *Electric Field Induced Glass Phases in Molecular Solids at Low Temperatures*, University of Florida, Physics

Watson, Brian C., *Quantum Transitions in Antiferromagnets and Liquid Helium-3*, University of Florida, Physics

Zhou, Kefei, *Thermodynamic Stability Study of DtxR H201W C-Terminal SH3 Domain*, Florida State University, Biological Sciences

REPORTS

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